2. Modeling the 2000 Episode

One of TCEQ's goals during the TexAQS was to select a new modeling episode for use in the upcoming Mid-Course Review[1]. The wealth of information collected during the study as well as the observed values of ozone and representative meteorological conditions led to the Photochemical Modeling Technical Review Committee's recommendation and TCEQ's selection of August 25 through September 1, 2000 as being an appropriate episode to model for Mid-Course Review in 2004. Details of the episode selection process are provided in Attachment 3. Negotiations with the BCCA-AG as a result of a lawsuit filed after the adoption of the December 6, 2000 SIP required TCEQ to perform an earlier Phase I Mid-Course Review with proposal by June 1, 2002. As a result, development of the 2000 episode was accelerated in hopes of using it to provide additional information regarding a possible VOC-NO_X tradeoff in the Phase I time frame.

2.1 Modeling enhancements

Numerous enhancements to meteorological and air quality modeling using the 2000 episode have been made since the December 6, 2000 SIP revision. Key among the improvements is the use of the state-of-the-science MM5 meteorological model. The MM5 modeling has been conducted by the Texas State Climatologist, Dr. John Nielsen-Gammon of Texas A&M University. The current meteorological input to the CAMx model is easily the most advanced and most representative episodic meteorological characterization for the HGA to date, additional work is ongoing to further enhance the meteorology for use in the upcoming Mid-Course Review. The MM5 modeling, which supports the air quality modeling performed with CAM-x, is summarized in Attachment 4 and is documented further in the supplemental technical reports produced by Dr. Nielsen-Gammon. The materials describe the current status of MM5 modeling as well as directions for future work.

The emissions inventory has also been upgraded in several ways. A special inventory from 81 industrial sources was collected, providing hourly emission rates and chemical speciation of VOC emissions. The on-road mobile source emissions were developed using EPA's MOBILE6, released in January 2002. The Texas Transportation Institute (TTI) used local travel-demand modeling results to develop detailed link-based inventories for the eight-county nonattainment area in both the 2000 base and 2007 future cases. Environ was contracted to upgrade the area source and nonroad emissions inventory based on more recent demographic information. These revised emission estimates have been incorporated into the modeling. The biogenic emissions inventory was developed using satellite radiation data along with GLOBEIS, a state-of-the-science model. The reader is referred to Attachment 5 for more details on developing the base and future year emissions inventories.

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[1]In this document, whenever the term "Mid-Course Review" is used, it refers to the upcoming 2004 Phase II Mid-Course Review unless otherwise noted. This document describes work conducted for the 2002 Phase I Mid-Course Review.

A new version of CAM-x is being used for the current modeling. CAMx-3 incorporates several enhancements over its predecessors, including multi-processor support, new analytical tools (process analysis and direct-decoupled method), flexi-nesting, chlorine chemistry, and more. The reader is referred to Attachment 1, the Modeling Protocol for a more detailed discussion of the advantages of CAMx-3.

One of the provisions of the BCCA-AG Consent Decree required TCEQ to issue a request for proposals for a peer view contractor. Envair was selected for this project. The peer review included a number of helpful suggestions, particularly concerning documentation, model performance evaluation, and certain categories of emissions development, but did not uncover any fundamental flaws in the model development. To the extent possible, these recommendations have been included in this document; additional recommendations will be incorporated into Phase 2 of the Mid-Course Review.

Since the original proposed SIP revision in June, 2002, the TCEQ staff and its contractors have made significant advances in understanding and improving the modeling characterization for the August 25 - September 1, 2000 episode. A number of improvements have been incorporated for the final adoption package, but many have not been included in the modeling demonstration directly for two reasons. First and foremost, the inclusion of gross changes to the model formulation could violate requirements for adequate public notice and require the package to be re-proposed. Second, several potential model enhancements are still in development and staff have not yet been able to confidently include these changes in the modeling. The TCEQ plans to incorporate many additional model improvements for Phase 2 of the Mid-Course Review.

2.2 The Modeling Domain

Figure 2-1 shows the modeling domain used for this analysis. The large modeling domain was chosen to reduce the influence of boundary conditions on the area of primary interest.

2.3 The August 25-September 1, 2000 base case

Once suitable meteorological and emissions inputs had been developed, the base case was run on the TCEQ's Silicon Graphics 16-processor modeling computer with two ramp-up days. These initial runs were conducted to perform installation testing of the modeling software and run scripts, and to provide an initial look at the model's performance. The first modeling runs used a preliminary inventory which included a 1999 point source inventory and MOBILE5-based on-road mobile source emissions, but it was apparent that the model was not producing enough

Figure 2-1: CAMx domain with nested sub-domains.

ozone. Even when the 2000 point source emissions (with a mostly-completed special inventory) and MOBILE-6 emissions were incorporated, modeled ozone concentrations fell far short of measured.

The TCEQ modeling staff conscientiously quality assure each modeling input file as it is developed. As an additional QA step, model inputs are reviewed in accordance with the Air Modeling and Data Analysis Section's Quality Assurance Plan. After the development of the base case emissions inventory was completed, the QA Plan was reviewed and assignments made to quality assure the work. The Quality Assurance Plan can be found in Appendix D, Protocol for Ozone Modeling of the Houston/Galveston Area: Phase I of the 2004 Mid-Course Review.

The causes of the poor initial model performance were reviewed, with several issues noted in both the meteorological and emissions inputs. One obvious candidate for the low ozone production was the reported point source emissions inventory, which had decreased markedly since the 1993 modeling. Point source VOC emissions decreased by over 50% and NO_X emissions dropped by nearly 30% compared with the 1993 base case. It is unclear how much of this change represents real reductions and how much is accounted for by so-called "paper" reductions, but it is clear from the TexAQS and subsequent analyses that the industrial VOC inventory is likely under-reported, which may explain partly the model's low ozone production. Other potential causes of model underprediction include modeled mixing heights which are higher than observed, timing of the sea breeze, and the simulation of a low-level nocturnal jet seen in the area.

A series of sensitivity analyses were conducted examining the various hypothesized causes for model underprediction. Several of the sensitivities involved increasing VOC and highly-reactive VOC (HRVOC)[2] emissions by various factors, ranging from three to more than an order of magnitude. One specific set of inventory modifications involved setting HRVOC emissions at several large HRVOC emitters equal to those facilities' NO_X emissions. This analysis was motivated by analysis of airborne NO_X and olefin measurements made by the Baylor Aircraft in 2001 near several industrial facilities in the area. Figure 1-13(a) presented earlier shows the flight path of one such flight, and Figure 1-13(b) plots concentrations of olefins and NO_Y. Note the collocation of the olefin and NO_Y plumes downwind of several facilities. In many of these collocated plumes, the concentrations of NO_Y and olefins are very similar, with olefin concentrations ranging from about half to approximately twice the NO_Y concentrations. The conclusion is that at least for several large olefin sources, olefin emissions are about equal to NO_X emissions (NO_Y consists of NO_X plus the photochemical reaction products of NO_X such as nitric acid).[3]

Some of the emission sensitivity runs were combined with meteorological sensitivities which modified the wind speed and planetary boundary layer thickness. A one-kilometer Flexi-nest grid covering the Ship Channel, Baytown, Texas City and most of Galveston Bay was included in some of the sensitivity runs. None of the individual changes produced adequate levels of ozone (except for one run in which the inventoried olefin emissions were increased by a factor of more than 30), but combining the planetary boundary level adjustments with an increased HRVOC emissions and flexi-nesting produced a model configuration which performed well on two days and produced acceptable high ozone concentrations on a third. This model configuration, referred to as Base1a.ks1f, was chosen for additional analyses including a test of the VOC-NO_X tradeoff discussed above. These results were presented in the June, 2002 proposed SIP revision.

The Base 1a configuration refers to modeling the 2000 point sources with most of the special inventory, along with MOBILE6 emissions in the 8-county nonattainment area. The ks1f designation indicates the particular set of model adjustments used: 30% reduction to the planetary boundary layer (pbl) also referred to a mixing height, use of the one-kilometer flexi-nest grid, and an adjustment to HRVOC emissions that set the mass of HRVOCs equal to the

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[2]For a list of compounds defined in this document as HRVOCs, see Attachment 5.

[3]Note that the actual emissions adjustment was applied to HRVOC emissions instead of olefin-only emissions, but the additional reactivity added to the modeled inventory was approximately the same.

mass of NO_X emissions at 26 selected large HRVOC emitting facilities in the HGA. Details of how the facilities were selected and how the adjustments were applied can be found in Attachment 5. The 30% reduction to the pbl was chosen after discussions with Dr. Nielsen-Gammon, who indicated that MM5 was simulating the pbl at about 30% higher than was seen by aircraft measurements.

Subsequent to the June, 2002 proposal, a number of changes have been incorporated into the modeling characterization, including:

Meteorology

Correction of a timing error in the profiler data used to "nudge" the MM5 wind fields. In the June modeling, this data had been incorporated with a discrepancy of approximately 1.4 hours between the profiler data and MM5. The most visible effect of this correction is to remove the time lag in ozone formation noted on August 25 in the Proposal.

Incorporation of upper-air wind data from the lidar instrument deployed at the La Porte airport during TexAQS 2000. Using this data helped to shift the location of the modeled peak ozone much closer to the observed peak than had been seen previously. Because the lidar data required extensive postprocessing to be used reliably, so far only the data for August 25 is available. The TCEQ plans to include data for other days when it becomes available.

Adjusting the hourly modeled pbl depth on August 30 to the average pbl observed by the radar profilers deployed during the TexAQS. This change helped reflect the delayed rise of the pbl on this day and increased peak ozone concentrations significantly. The TCEQ staff are developing a more broad-based application of the profiler data to adjustment of the modeled pbl, but the results of this approach were not available in time to be included in the modeling discussed in this document.

Emissions

The latest model formulation now includes link-based Mobile 6 emissions in Beaumont-Port Arthur, instead of the county-level data used previously. Additional enhancements to the mobile source emissions in the remainder of the modeling domain will be included in Phase 2 of the Mid-Course Review modeling.

The model now includes emissions from Mexican sources developed as part of the BRAVO modeling effort.

Point sources throughout the modeling domain now use hourly emissions from the Acid Rain data base. In the modeling included in the June proposal, only Texas and Louisiana sources used this data.

New area source emissions, developed for the 1999 Periodic Emissions Inventory are now available and have been incorporated into the modeling. Some non-road mobile source emissions have also been updated.

Improved hydrocarbon speciation from the PSDB and Special Inventory has been incorporated into the point source emissions. This step is important in assessing the contributions of various sources to emissions of HRVOCs.

Additional quality assurance of the point source special inventory has resulted in numerous corrections, and has allowed most of it to be included in the modeling in its entirety.

A chlorine inventory for the August 25- September 1, 2000 has been developed, but has not yet been included in the modeling. Chlorine chemistry will be employed in modeling conducted for the Mid-Course Review.

Note that none of the emissions changes incorporated since June, 2002 have had a dramatic influence on the modeling. They are included at this time because they are part of the ongoing effort by TCEQ to continually improve its modeling and regulatory inventories.

In the June, 2002 SIP proposal, both base case and future case modeling was only reported for the "adjusted" base case (Base1.ks1f) which included both the 30% pbl reduction and the HRVOC-to-NO_X adjustment to point source emissions. Because EPA considers these adjustments to be sensitivity analyses (even though they are both reasonable and based on aerometric measurements), in this document we will present results for both the "unadjusted" and "adjusted" base cases. The new "unadjusted" base case, referred to as Base4a.regular, includes all modifications above except the profiler-based adjustment on August 30. The "adjusted" base case, which includes a 30% pbl reductions on all days except August 30, the profiler-based pbl adjustment on August 30, and the HRVOC-to-NO_X adjustment to point source emissions, is referred to hereafter as Base4a.pt_o2n2_070pbl, or simply the adjusted base case.

Because the final modeling configuration for the December adoption package was not completed until late October, 2002, it was not possible to re-run all relevant analyses using the latest model configurations. Consequently, some results in this document and its attachments were conducted using earlier model configurations. Whenever results from earlier configurations are reported, the version will be noted.

Table 2-1 below summarizes the Base4a.regular and Base4a.pt_o2n2_070pbl emissions in the 8-county nonattainment area for August 30, both before and after adjusting the HRVOC emissions.

Table 2-1: Base Case emissions in the eight HGA nonattainment counties, Aug. 30, 2000

Emissions category		Emissions (tons/day)	
		NO_X	VOC[1]
On-road mobile		246	156
Area/Nonroad mobile		193	241
Point	unadjusted (Base4a.regular)	490	178
	adjusted (Base4a.pt_o2n2_070pbl)	490	327
Biogenic		21	1713
8-County Total	unadjusted (Base4a.regular)	950	2286
	adjusted (Base4a.pt_o2n2_070pbl)	950	2437

[1] Note that the VOC values reported here are the Carbon-Bond IV hydrocarbon masses used by CAMx and differ slightly from the actual masses.

2.4 Base case model performance evaluation

Table 2-2 shows model performance statistics for the unadjusted base case, including the August 24 ramp-up day (model performance was poor on the first two ramp-up days even with meteorological and inventory adjustments). The statistics are calculated for monitors in the eight HGA counties only. Note that September 1, 2000 was not modeled as part of the Base4a series of model runs. This day suffered from serious model performance problems, and to conserve both staff and computing resources it was decided to halt the modeling analysis a day early. The TCEQ will continue to analyze September 1, and if possible include modeling for that day in the Mid-Course Review. Note that the peak observed values in the table have changed since the June 2002 proposal due to inclusion of monitored ozone concentrations at the La Porte airport.

Table 2-2: Base4a.regular model performance in HGA 8-county area (4 km grid)

Statistic	EPA range	Date							
		8/24	8/25	8/26	8/27	8/28	8/29	8/30	8/31
Normalized Bias (%)	< +/-15	-28.5	-35.1	-12.6	2.9	5.6	-13.1	-11.6	-1.1
Normalized Gross Error (%)	< 35	30.3	37.4	17.4	7.0	12.5	18.8	20.1	13.7
Peak Observed (ppb)		120	194	140	87	112	146	201	176
Peak Pred (ppb)		89	113	115	97	104	102	108	133
Accuracy of Peak (%)	< +/-20	-26.1	-42.0	-18.2	11.4	-7.4	-30.3	-46.2	-24.0

The normalized bias figures in Table 2-2 show that the model generally underpredicts ozone concentrations on August 24 and 25. Although the model produces acceptable levels of bias thereafter, substantial underprediction is still seen on August 26, 29, and 30. Normalized gross error is quite large on August 24 and 25, primarily owing to the large biases on those days. The model shows moderate gross error for the remainder of the episode.

The major performance issue is the model's inability to produce peak ozone concentrations approaching the high monitored values on August 25, 29, 30, and 31. In fact, the only day in which an exceedance of the NAAQS was simulated was August 31, with no other day predicting ozone peaks over 110 parts/billion. In general, the model appears to be simulating ozone concentrations reasonably well when the monitors recorded low-to-moderate ozone, but fails to reproduce the highest values.

After running numerous sensitivity analyses, the TCEQ staff picked a model configuration that was both based on measured aerometric data and performed well for the days of primary interest: August 25, 29, 30 and 31. When the pbl and emissions adjustments described above are employed, model performance improves substantially for the four days of primary interest. Table 2-3 shows model performance for the Base4a.pt_o2no_070pbl base case for the 4-km grid, and Table 2-4 shows model performance in the 1-km flexi-nest grid only. Note that the 1-km grid was only used on August 25 and 29-31.

Table 2-3: Base4a.pt_o2n2_070pbl model performance in HGA 8-county area (4 km grid)

Statistic	EPA range	Date							
		8/24	8/25	8/26	8/27	8/28	8/29	8/30	8/31
Normalized Bias (%)	< +/-15	-15.0	-15.6	-3.6	18.6	22.4	-2.5	-11.3	1.9
Normalized Gross Error (%)	< 35	22.3	33.8	16.7	19.3	25.8	20.9	21.8	14.3
Peak Observed (ppb)		120	194	140	87	112	146	201	176
Peak Pred (ppb)		107	198	142	124	128	156	149	161
Accuracy of Peak (%)	< +/-20	-10.5	2.0	1.5	42.1	14.1	7.1	-25.7	-8.4

Table 2-4: Base4a.pt_o2n2_070pbl model performance in 1-km flexi-nest grid

Statistic	EPA range	Date			
		8/25	8/29	8/30	8/31
Normalized Bias (%)	< +/-15	-17.2	2.4	-10.7	2.7
Normalized Gross Error (%)	< 35	34.3	22.6	23.6	14.3
Peak Observed (ppb)		194	146	201	176
Peak Pred (ppb)		209	160	161	173
Accuracy of Peak (%)	< +/-20	7.6	9.6	-19.7	-1.7

Overall, model performance with the Base4a.pt_o2n2_070pbl is seen to be much better than seen with the unadjusted (Base4a.regular) base case. Model performance with the adjusted base case now meets the minimum EPA statistical requirements on August 26, 29, and 31 using the 4-km grid, and meets performance specifications on August 29, 30, and 31 when using the flexi-nest grid (note August 26 was not run with flexi-nesting). Additionally, model performance for August 25 narrowly misses because of general underprediction of ozone, even though the peak on that day is larger than observed. The major performance issue on August 25 appears to be a northerly displacement of the modeled ozone from the area in western Harris County where the majority of ozone exceedances were recorded that day. Had the modeled winds been a rotated a few degrees counterclockwise, it is likely that model performance would have been quite good on August 25. Figure 2-2 show peak daily modeled ozone in the 4-km grid for August 25, for both the unadjusted and the adjusted base cases. Clearly, the latter model configuration reproduces the measured ozone peaks better than the former.

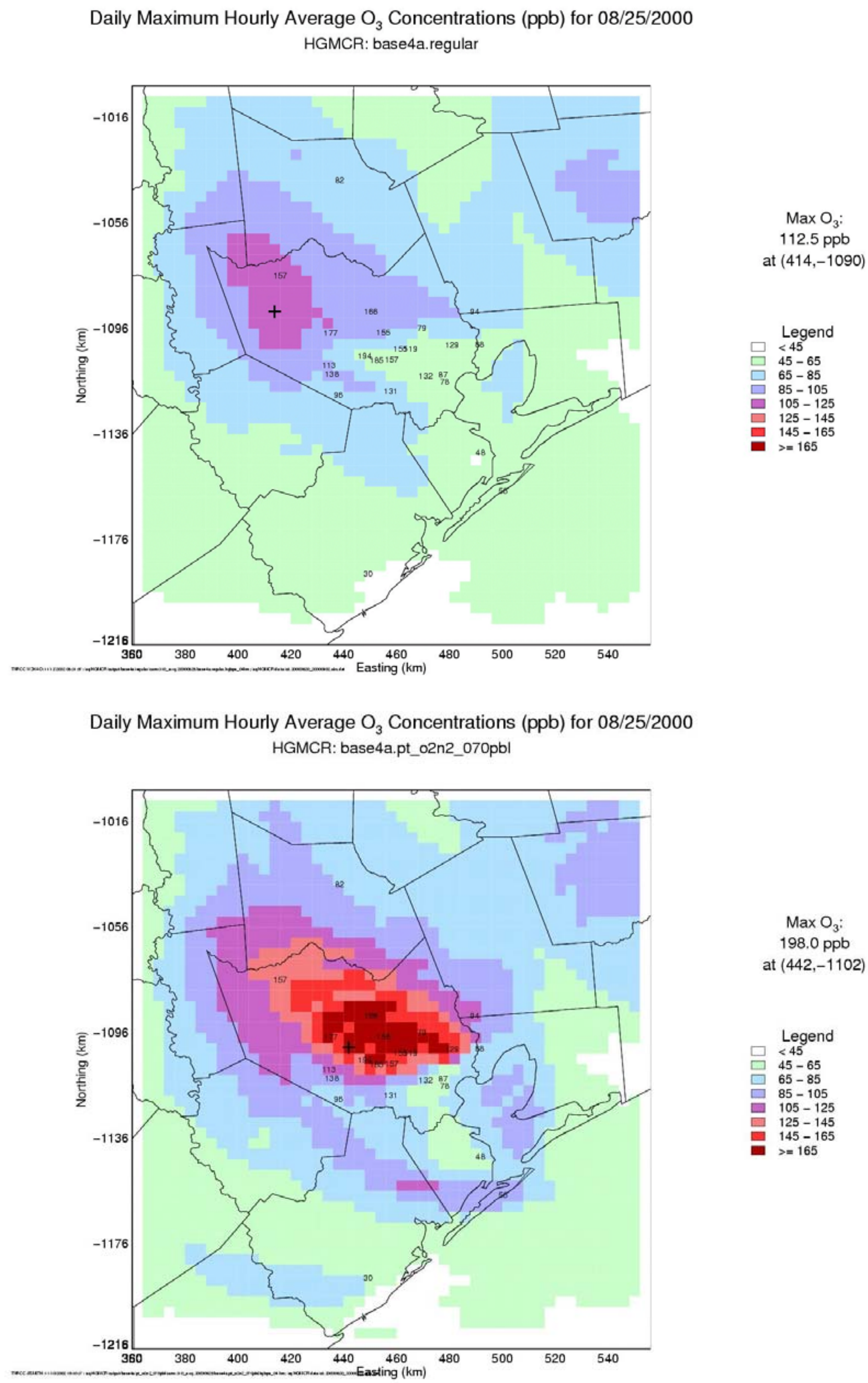


Figure 2-2: Peak modeled ozone concentrations on August 25, unadjusted (top) and adjusted (bottom) base cases.

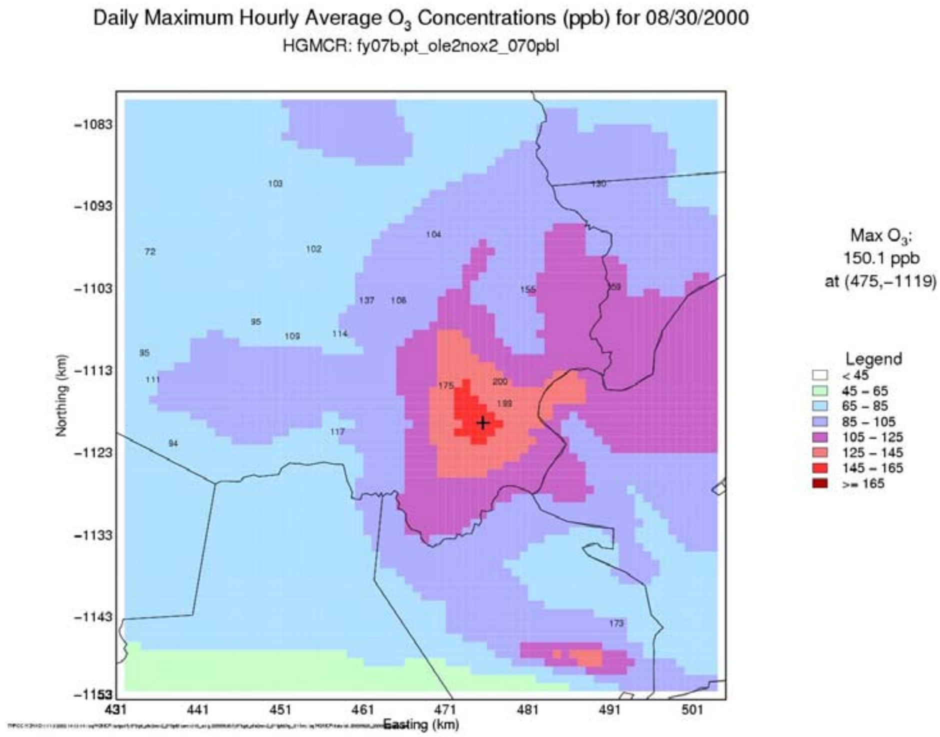
For a detailed discussion of model performance, including daily maximum ozone plots and time series for both Base4a.regular and Base4a.pt_o2n2_070pbl, see Attachment 6. The remainder of this section describes some of the sensitivity analyses conducted primarily to improve model performance on August 30. Although the performance for this day was acceptable (using flexi-nesting), the model showed a significant bias towards underprediction. Part of the underprediction may be explained by two events observed that day indicated that additional emissions adjustments were warranted. First, a large flare was observed for several hours that day in the Channelview area (see Figure 2-3). Second, an aircraft canister collected that day near the La Porte airport showed extremely high concentrations of several HRVOCs. Back trajectory analysis placed the source of these HRVOCs in the western Ship Channel area. A complete analysis of the canister and its likely origins are described in the next section of this document.

Figure 2-3: Smoking flare observed on August 30, 2000

Sensitivity analyses conducted on earlier versions of the base case indicated that these events were apparently independent, so separate adjustments were applied to Base4a.pt_o2n2_070pbl to account for them. First, the flare was identified, and its reported emissions from the Special Inventory were increased by a factor of 10. This factor corresponds to a reduction in the flare's assumed destruction efficiency from 99% to 90%, which is in the range of destruction efficiencies measured in flare testing for unstable flame operation during EPA flare testing. A summary of those tests are found in two reports entitled Evaluation of the Efficiency of Industrial Flares: Test Results, May 1984 (EPA resport number 600/2-84-095) and Evaluation of the Efficiency of Industrial Flares: Flare head Design and Gas Composition, Sept 1985 (EPA Report Number 600/2-85/106). Note that the picture actually shows two flares, one of which was burning brightly but not smoking. Second, analysis of the airborne canister compared to measurements of NO_Y made at the same time indicated that emissions of the sampled HRVOCs were approximately 1.5 times the NO_X emissions. A set of seven upwind accounts were identified, and their emissions for August 30 were increased by an additional 50% to simulate this observation.

Additionally, analysis by Dr. Harvey Jeffries indicated that the modeled emissions of NO_X from mobile sources might be overstated by as much as 30%. Analysis by TCEQ staff of the MOBILE6 ABSOLUTE HUMIDITY input indicated that emission corrections for humidity are only applied to the light-duty gasoline portion of the vehicle fleet. If similar adjustments are applied to the heavy-duty gasoline and diesel portions of the fleet, then on-road NO_X emissions from the entire fleet would be expected to decrease by approximately 10% from currently estimated levels. Similarly, emissions of NO_X from non-road sources might experience a similar decrease when adjusted for the high humidity normally seen in the HGA. However, the current version of the NONROAD model does not apply emission corrections based on humidity inputs. Hence, in addition to the two point source adjustments discussed above, NO_X emissions from on-road mobile sources were therefore decreased by 25% (nonroad sources were not adjusted separately, but it may be assumed that some portion of the adjustment to on-road emissions serves as a surrogate for non-road emissions). The model configuration with the above modifications is called Base4a.pt_o2n2bs10a_m075n_070pbl.

Figure 2-4 shows August 30 peak modeled ozone concentrations for the 1-km flexi-nest grid for both the adjusted base (Base4a.pt_o2n2_070pbl) and sensitivity (Base4a. pt_o2n2bs10a_m075n_070pbl) model runs. Clearly, modeled prediction of peak ozone, which occurs downwind from the highly-reactive canister sample, has improved markedly both in magnitude and location. Also, the underestimation at monitors in the northeastern portion of the 1-km grid, downwind from the smoking flare, is improved significantly. Finally, the general underprediction of peak ozone in west-central portion of the domain (urban core) is improved. The three reasonable additional modifications to the modeled emissions are seen to produce excellent model performance for August 30.



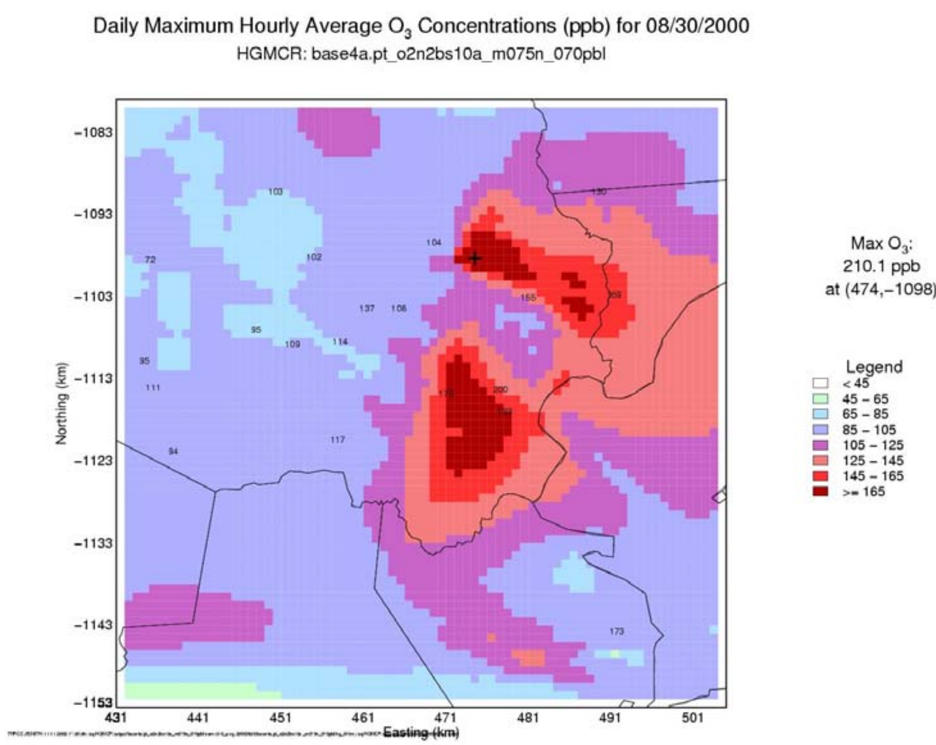


Figure 2-4: August 30 peak modeled ozone for adjusted base case (top) and sensitivity base case (bottom)

Table 2-5 shows model performance after making the changes described above. The only change made to August 25, 29, and 31 was the 25% decrease in mobile emissions.

Table 2-5: Base4a.pt_o2n2bs10a_m075n_070pbl model performance in 1-km flexi-nest grid

Statistic	EPA range	Date			
		8/25	8/29	8/30	8/31
Normalized Bias (%)	< +/-15	-14.5	4.8	-4.7	1.4
Normalized Gross Error (%)	< 35	33.5	20.7	20.4	14.6
Peak Observed (ppb)		194	146	201	176
Peak Pred (ppb)		209	156	210	160
Accuracy of Peak (%)	< +/-20	7.9	7.1	4.8	-9.1

Overall, the changes made in this sensitivity did not dramatically affect model performance except for August 30, were the bias is much better and the modeled peak closely matches the measured peak in magnitude. The location of the modeled peak has shifted from the Deer Park area to the Channelview area, immediately downwind from the smoking flare, but the model actually predicted a peak of 197 ppb approximately five kilometers from the observed peaks at La Porte airport (201 ppb) and at HRM 4 (199 ppb).

Many other sensitivity analyses were conducted after June, 2002, and are listed in tabular format in Appendix B. One analysis included two modifications of particular interest: applying an hourly adjustment to the modeled pbl for all days, and using a HRVOC adjustment scheme based on data collected at five automatic gas chromatographs deployed near the Ship Channel. When this configuration was modeled in late October of 2002, overall performance was consistently poorer than was seen with the Base4a.pt_o2n2_070pbl base case. Because of time constraints and also because of public-notice considerations, no attempt was made to further develop this base case for the current analysis. However, both of the modifications described are technically supportable and will be investigated fully for possible inclusion in the Mid-Course Review modeling.

2.5 Future case modeling

The modeling inventory developed for 2007 includes all the rules adopted to date with two exceptions. Energy efficiency, a so-called "gap measure" adopted in the December, 2000 SIP revision, was not modeled because the effects will primarily occur at electric generation units, but without performing sophisticated supply-demand modeling, it is impossible to specifically determine at which units the reductions will be realized. Also, reductions due to rules intended to permit all grandfathered sources in Texas (HB 2912) were not modeled because the TCEQ New Source Review program will not be able to complete its analysis of the effects of these rules until it receives permit applications from the affected entities (due by September, 2003 for East Texas). Anticipated activity growth was applied to area, on-road mobile, and nonroad mobile sources, along with any applicable state and federal regulations. Point source emissions were not "grown" *per se,* since TCEQ point source trends analyses have demonstrated that there has been essentially no growth, or negative activity growth, in most regions of the state.

For NO_X emissions, the 2007 nonattainment area-wide cap was obtained from the TCEQ Banking and Trading program. The 2007 emission limit was calculated by adding to the cap all banked emissions expected to be used in 2007. Electric Generation Units (EGUs) were assumed to operate at their specified Emissions Specifications for Attainment Demonstration (ESADs), while non-EGU emissionss were reduceded uniformly until the total emissions of EGUs and non-EGUs was equal to the calculated 2007 emission limit. A limited number of small source categories did not have specified ESADs; these sources were assumed to operate at 2000 levels in 2007. For VOC emissions, no chages were assumed from 2000 to 2007, except that banked emissions were added to the 2007 emissions, resulting in a slight amount of growth for the VOC sources. The development of the future-case emissions is described in more detail in Attachment 5.

In general, the rules modeled were similar to those modeled in the December, 2000 SIP Revision. The following list describes some of the controls modeled; for a complete description of the 2007 future case see Attachment 5.

- The future case inventory includes the point source NO_X reductions adopted in December, 2000 (the "90%" reductions), except that emission limits for HGA electric generation facilities were modified as per ESAD revision, September 2001.
- The VMEP reductions were included as calculated in the December, 2000 SIP Revision. In future modeling, the on-road portion of VMEP will be re-calculated using MOBILE6.
- The construction delayed start time was not modeled. In its place, we modeled the equivalent NO_X reductions which are expected to occur under the TERP.
- An eight-county 55 mph speed limit was modeled. Although the speed limit was recently increased beyond 55 mph, the current regulations call for its re-imposition unless equivalent reductions can be found by 2007.

Table 2-6 shows future case emissions for both the unadjusted future case (called fy07b.regular), built from the Base4a.regular base case and an adjusted future case (called fy07b.pt_o2n2_070pbl), developed from the base4a.pt_o2n2_070pbl base case.

Table 2-6: Future Case emissions in the eight HGA nonattainment counties, Aug. 30, 2000

Emissions category		Emissions (tons/day)	
		NO_X	VOC[1]
On-road mobile		129	86
Area/Nonroad mobile		156	215
Point	unadjusted (fy07b.regular)	87	182
	adjusted (fy07b.pt_o2n2_070pbl)	87	331
Biogenic		21	1713
8-County Total	unadjusted (fy07b.regular)	393	2196
	adjusted (fy07b.pt_o2n2_070pbl)	393	2345

[1] Note that the VOC values reported here are the Carbon-Bond IV hydrocarbon masses used by CAMx and differ slightly from the actual emissions.

Table 2-7 shows the peak modeled ozone levels for each day with both the unadjusted and adjusted emissions. For the adjusted case, results for the 1-km flexi-nest grid are also shown.

Table 2-7: Modeled 2007 daily peak modeled ozone concentrations

Case	Grid	Episode day							
		8/24	8/25	8/26	8/27	8/28	8/29	8/30	8/31
fy07b.regular	4 km	89	113	97	79	89	91	102	113
fy07b.pt_o2n2_070pbl	4 km	107	188	117	94	108	152	146	136
	1 km		201				164	150	142

2.6 VOC substitution modeling

After developing a suitable future case, the next step in the modeling process was to determine how much reduction in VOC emissions would - given that alternate ESADs (nominal 80% NO_X reductions) are adopted - be necessary to achieve the same air quality benefit as the original ESADs (nominal 90% NO_X reductions). To address this issue, a second version of the 2007 adjusted inventory was prepared, but this time applying alternate ESADs to the point sources (see Attachment 5 for details on modeling the alternate ESADs). Then two additional modeling inventories were developed, both using the alternate ESADs. The first included half of the additional HRVOC emissions and the second contained no extra HRVOC emissions. Note that the modeling discussed in this section was conducted with an earlier version of the future case (fy07a) than that discussed in the previous section. The primary difference in the two future cases is that the fy07b case includes approximately 8 more tons/day of point source NOx in

HGA than the fy07a case, in order to more closely simulate the expected 2007 HGA NOx emissions.

Table 2-8 displays the daily peak ozone concentrations from the series of model runs described in this section. The second column shows the base case (Base4a.pt_o2n2_070pbl) peak ozone, while the third gives the future case peaks, assuming currently adopted controls. The fourth through sixth columns show the peak under alternate ESAD controls combined with various reductions to the additional HRVOC emissions. The fourth column includes all added HRVOC emissions, while the fifth column includes half the added HRVOC emissions. The fifth column then represents a reduction from the fourth column of half the added HRVOC's, which amounts to a 39% reduction in the total amount of HRVOC emissions. The last column similarly represents a reduction of 78% from the total HRVOC emissions represented in column four.

Table 2-8: Summary of NO_X/VOC equivalence modeling

	Peak Ozone (parts/billion)					
		2007 Future Case				
			Alternate ESADs ("80%" NO_X reduction)			
Episode day	Adjusted 2000 Base Case	Current Point Source NO_X Reduction ("90%")	No new VOC reductions	"39%" HRVOC reduction	"78%" HRVOC reduction	Required HRVOC reduction (%)
8/25	209	195	206	181	140	17.2
8/29	160	159	169	144	114	15.6
8/30	161	146	156	145	131	**35.5**
8/31	173	142	147	137	126	19.5

Notes:

- Peak ozone values on August 25 were reprocessed to remove "spikes" seen at 07:00. For details, see Attachment 6.
- The peak ozone values were based on the fy07a series, hence the values listed under "Current Point Source NO_X Reduction ("90%")" differ slightly from the fy07b series results presented in the last section.

Starting with the alternate ESAD case ("80%")including 100% of the added HRVOC's, we can calculate the ozone benefit accrued by applying the more stringent reductions of the December, 2000 SIP revision ("90%") by simply calculating the difference in peak modeled ozone between the two runs. In this table, the benefit of increasing point source NO_X reductions from "80%" to "90%" is found by subtracting the concentration in column 3 from that in column 4. For example, on 8/29 the benefit of the "last 10%" of NO_X reductions is 169-159 = 10 ppb. Next, the benefit of a 39% reduction from HRVOC emissions is found by subtracting the concentration in the fifth column from that in the fourth. Again for August 29, the benefit is then 169-144 = 25 ppb. So under the current inventory assumptions, a 39% reduction in HRVOC emissions would be 2.5 times more beneficial than the last 10% of point source NO_X reductions on August 29. Interpolating gives the value in the last column of the table, which is the percentage reduction required in emissions of HRVOCs to provide the same ozone benefit as the last 10% of NO_X emissions.

The value in bold typeface in Table 2-8 (35.5%) occurs on August 30 and is the largest percentage requirement. Thus 36% (rounded) represents the minimum required reduction to HRVOC emissions that must be achieved in order to demonstrate equivalence.

As with the base case, the TCEQ modeling staff conscientiously quality assured each modeling input file as it was developed, and future-case model inputs were reviewed in accordance with the Air Modeling and Data Analysis Section's Quality Assurance Plan (see Appendix D).

In conclusion, modeling with the August 25-September 1, 2000 episode indicates that it is possible to achieve an equivalent air quality benefit with some level of HRVOC reductions in lieu of some or all of the last 10% of the currently required NOx emissions. Furthermore, a reduction of approximately 36% in emissions of highly-reactive volatile organic compounds appears to be sufficient to provide equivalence. These conclusions are based on the strongly supportable assertion that emissions of HRVOCs are much larger than reported in the inventory, but the method used to adjust the inventory to include these unreported emissions should be considered a first-order approximation and will be refined in future work. In any case, it is clear that additional reductions will be necessary to bring the area into attainment of the NAAQS for ozone.

2.7 The future control case

Based on the results presented in the preceding section, the TCEQ developed a control strategy which will provide greater air quality benefits than those achievable with controls propagated in previous SIP revisions. Together with the alternate ESADs (the "80%" NO_X reductions), this new strategy targets four highly-reactive VOC categories: ethylene, propylene, 1,3-butadiene, and butenes. All four HRVOCs will be reduced in Harris County, while the remaining counties will have reductions in only the two most important, ethylene and propylene.

As seen in the previous section, it is necessary to reduce emissions of HRVOCs by at least 36% to achieve the same benefit as the "last 10%" of NO_X reductions (based on the fy07a model configuration - slightly more reduction would be required using fy07b). The current strategy will reduce HRVOC emissions in Harris County by approximately 50% (on a reactivity basis), and will significantly reduce HRVOC emissions in the remaining seven counties in the nonattainment area.

The following pie chart (Figure 2-5) shows reported 2000 emissions of HRVOCs in the greater Ship Channel area (including Channelview, Mount Belview, and Bayport), weighted by Maximum Incremental Reactivity (MIR), a measure of each compound's ozone-forming potential (Carter, W. P., 2000). This chart shows that ethylene and propylene emissions account for more than half of the reactivity associated with HRVOC emissions in the Ship Channel area.

Additionally, butene and 1,3 butadiene emissions account for nearly one quarter of the reactivity. By reducing emissions of these four HRVOCs by 64%, the overall reactivity of the HRVOCs will be reduced by 50%.

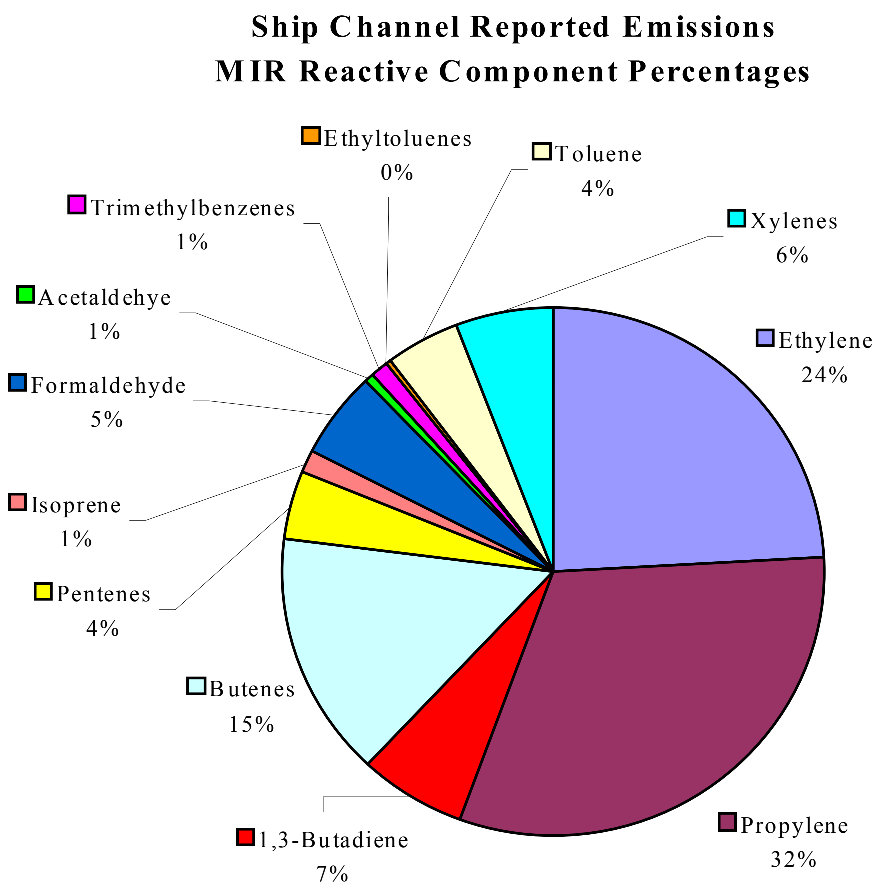


Figure 2-5: Reactivity-weighted emissions of HRVOCs in the greater Ship Channel area

To model the effects of these reductions, the TCEQ modeling staff started with the adjusted fy07b future case, with the alternate ESADs. Reductions were then applied to the added HRVOC emissions to achieve the required total reduction (for example, reducing the extra HRVOC emissions by 63% results in an overall HRVOC emission reduction of 50% in Harris County). Note that the additional HRVOCs were not modeled specifically; the additional HRVOCs were simulated by adding emissions of two Carbon-Bond IV species (ETH and OLE, 40% and 60% respectively). This mixture is representative of olefin emissions, which comprise the bulk of the HRVOCs, but may not accurately represent all compounds in the original list of HRVOCs. However, since all the reductions called for in this SIP revision apply to olefins, the effect of these reductions should be represented adequately in the modeling analysis.

Table 2-9 below compares (adjusted) point source emissions for the new 2007 control case with the original 2007 case ("90%" NO_X reductions). Attachment 8 shows how the modeled HRVOC emissions, before and after controls, were distributed among source categories in Harris County and separately in the surrounding seven counties. Table 2-10 shows peak simulated ozone for the four episode days of primary concern, and also shows additional metrics which provide more comprehensive measures of ozone exceedances than the daily peak. These additional metrics are: geographic area where ozone exceeded 125 parts/billion on that day, area-hours (geographic area weighted by the temporal extent of the exceedance), and area-hours-ppb, which accounts for area-hours but in addition weights the measure by the amount by which the ozone concentration exceeded 125 parts/billion.

Table 2-9: Adjusted Future Case point source emissions in the eight HGA nonattainment counties, Aug. 30, 2000, for old and new control strategies

Control strategy	Emissions (tons/day)	
	NO_X	VOC[1]
Old ("90%" NO_X reduction, no VOC reduction)	87	331
New ("80%" NO_X reduction plus HRVOC reductions)	143	249

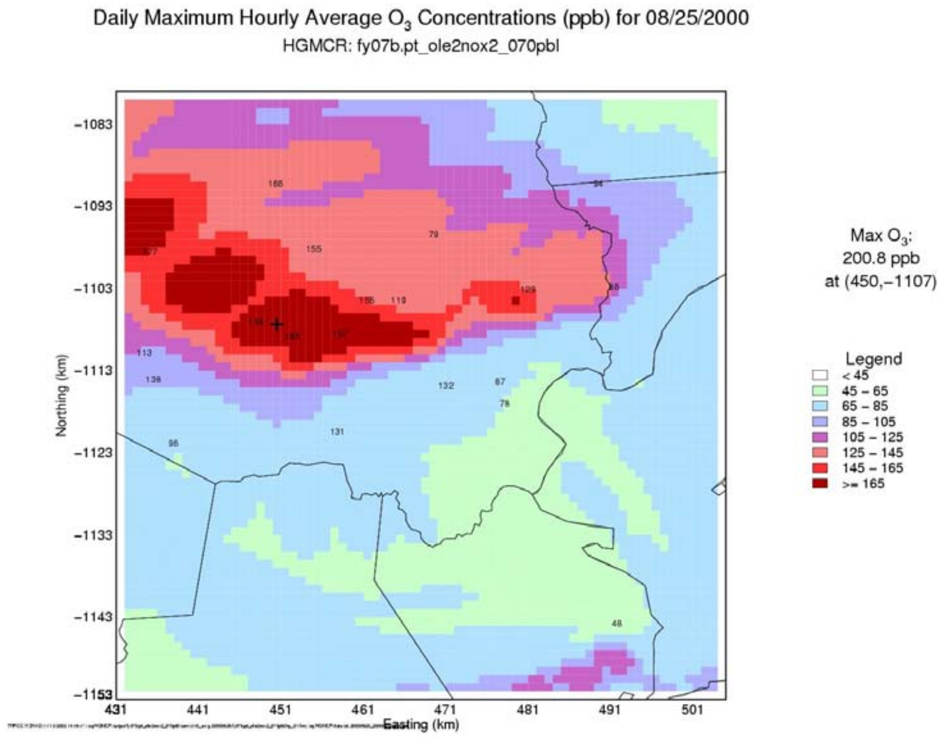
[1] Note that the VOC values reported here are the Carbon-Bond IV hydrocarbon masses used by CAMx and differ slightly from the actual masses.

Table 2-10: Comparison of ozone metrics between old and new control strategies.

Metric	Control strategy	Episode day			
		August 25	August 29	August 30	August 31
Peak ozone (parts/billion)	Old	201	164	150	142
	New	175	134	144	136
Geographic area of exceedance (km^2)	Old	1629	277	198	195
	New	1199	48	107	97
Area-hours (km^2-hr)	Old	2340	346	484	266
	New	1380	49	222	120
Area-hours-ppb (km^2-hr-ppb)	Old	38589	3257	4324	1469
	New	16528	187	1604	386

For all days and all metrics, the new strategy is seen to provide much greater air-quality benefits than its predecessor. Although peak ozone remains above the 125 parts/billion standard for all days, the new strategy provides reductions of between 6 and 30 parts/billion compared to the old strategy. In fact, on the two best performing days, August 29 and 31, the modeled ozone peak is now in the mid 130's. Geographic area of exceedance is reduced between 26% (on August 25) and 83% (on August 29) with the new strategy. The new strategy reduces area-hours by between 41% (on August 25) and 86% (on August 29) compared with the old strategy. The most comprehensive metric, area-hours-ppb, shows the greatest reductions, ranging from 57% on August 25 to 94% on August 29.

Figures 2-6 through 2-9 show side-by-side comparisons of daily peak ozone with both the old and new control strategies for the one-kilometer flexi-nest grid. The differences noted in the table above are readily apparent from the figures.



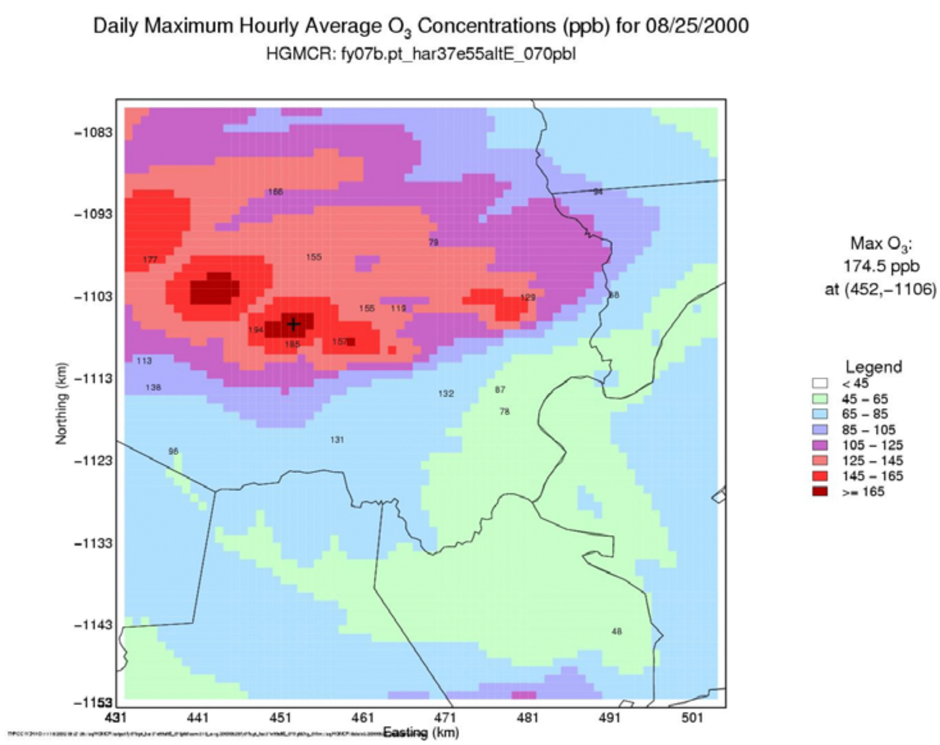
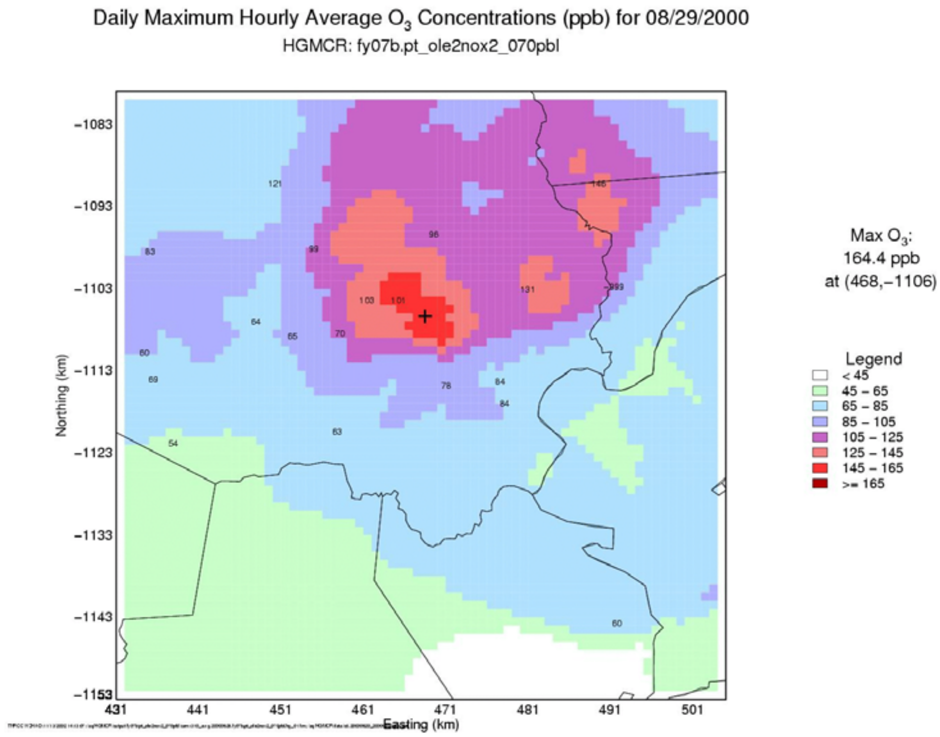


Figure 2-6: Peak modeled ozone concentration on August 25, old control strategy (top) compared with new strategy (bottom)



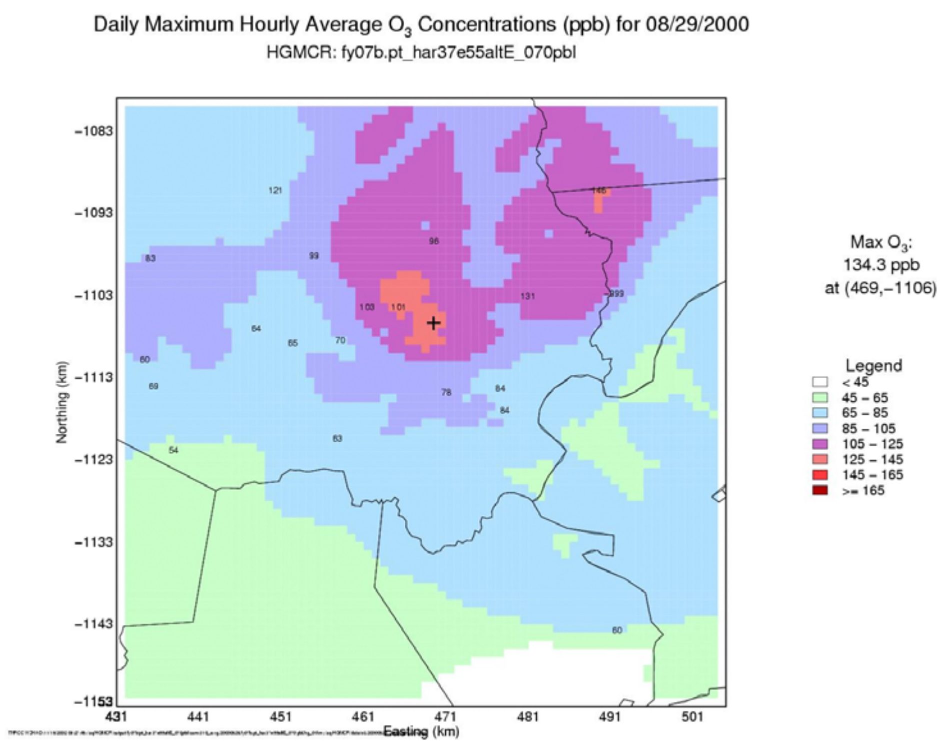


Figure 2-7: Peak modeled ozone concentration on August 29, old control strategy (top) compared with new strategy (bottom)

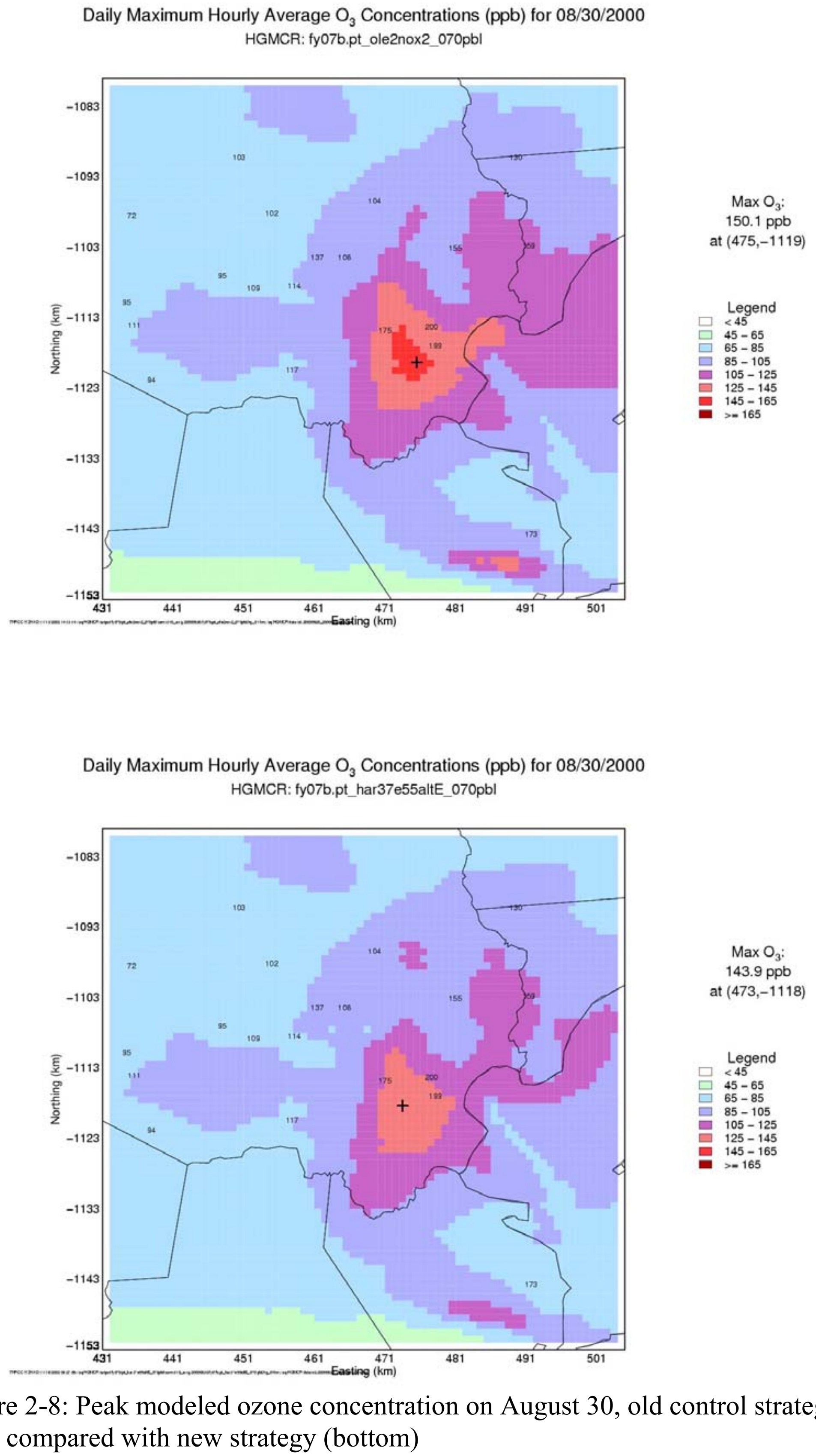
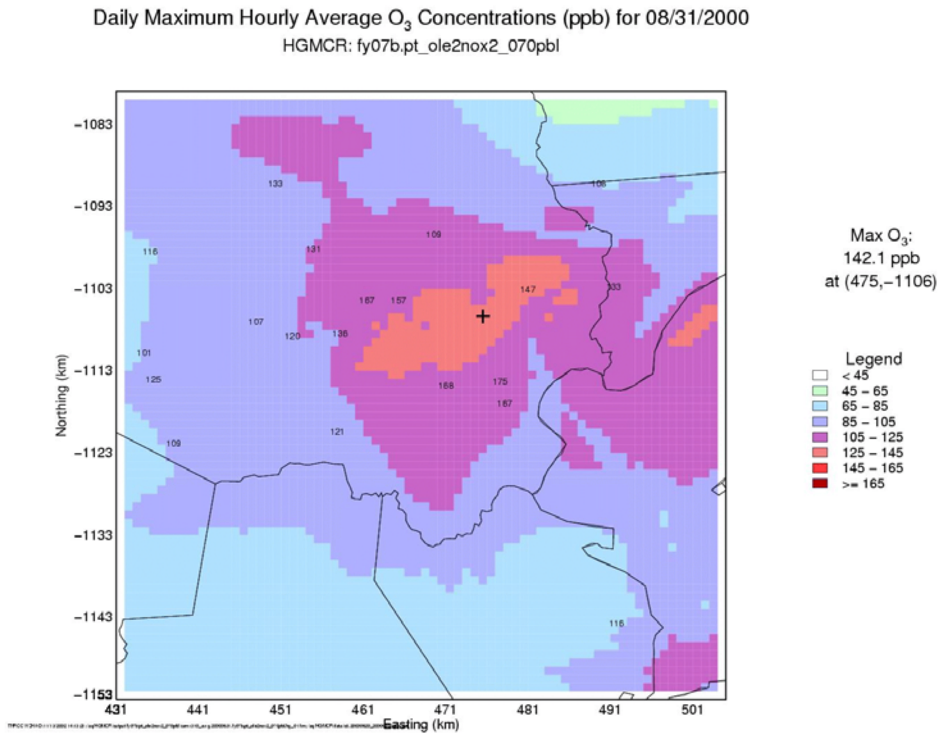


Figure 2-8: Peak modeled ozone concentration on August 30, old control strategy (top) compared with new strategy (bottom)



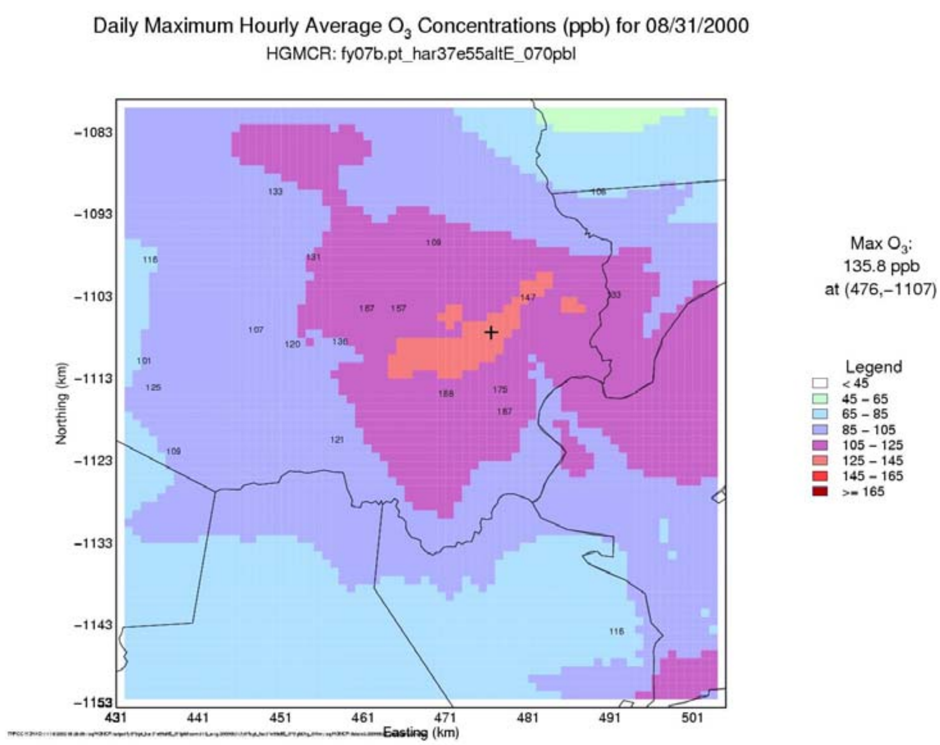


Figure 2-9: Peak modeled ozone concentration on August 31, old control strategy (top) compared with new strategy (bottom)

Note that the new control strategy does not include the so-called “gap” measures that had not yet been identified as of December, 2000. These reductions amount to 56 tons/day of additional reductions in emissions of NO_X, but have not been identified with specific sources or even categories of sources. To model these reductions, the future controlled NO_X emissions were reduced an additional 56 tons/day across-the-board, with reductions taken from all anthropogenic sources of NO_X. In addition, NO_X reductions of 3.6 tons/day from energy efficiency were included (this “gap” measure was identified in the December 2000 SIP revision, but was not included in the future control strategy modeled above, since it is difficult to associate these reductions with specific sources). Table 2-11 below compares the various ozone metrics from this control strategy run with the “New” control strategy described above.

Table 2-11: Ozone metrics for new control strategy, with and without additional “gap” reductions in NO_X emissions.

Metric	Additional “gap” reductions?	Episode day			
		August 25	August 29	August 30	August 31
Peak ozone (parts/billion)	Without	175	134	144	136
	With	173	138	139	132
Geographic area of exceedance area (km^2)	Without	1199	48	107	97
	With	896	48	89	41
Area-hours (km^2-hr)	Without	1380	49	222	120
	With	1055	49	172	45
Area-hours-ppb (km^2-hr-ppb)	Without	16528	187	1604	386
	With	13050	242	975	97

From the table, it is seen that the additional “gap” reductions are expected to have relatively minor effects on peak ozone. Modeled peak ozone concentrations are lowered by up to 5 parts/billion on August 25, 30 and 31, but a disbenefit is seen on August 29. All metrics respond better to the additional reductions on August 30 and 31 than on the first two days, with dramatic improvements seen on August 31.

In the December 2000 SIP revision, the “gap” calculation was made to estimate the amount of NO_X reductions necessary to reach attainment. However, even with all “gap” measures accounted for in the current modeling, future ozone concentrations are still above the standard on all days. Considering the significant adjustment made to the VOC emissions in the current modeling, it is not surprising that future-case ozone concentrations are higher than those predicted in December of 2000, since significant amounts of HRVOC emissions remain in the system even after the considerable reductions attributable to the new control strategy. Clearly additional reductions to emissions of NO_X, VOC, or both will be necessary to reach attainment by 2007. The next section describes a modeling analysis that provides guidance on which types of additional reductions will be most effective.

2.8 Directional guidance analysis

Once the final control strategy was developed, the TCEQ modeling staff began a series of model runs designed to provide directional guidance about further reductions necessary to reach attainment.

The runs represent a series of across-the-board reductions to anthropogenic emissions, starting with the 2007 controlled inventory (not including the additional "gap" measures). These reductions, in increments of 25%, are applied equally to all sources and do not necessarily represent any potential control strategy. Also, the runs do not differentiate among source types or among emitted species. Therefore, specific control strategies may be much more effective than across-the-board reductions. For example, additional reductions targeted at HRVOCs will likely be, ton for ton, much more effective in reducing ozone than reductions spread evenly among all VOC sources. Similarly, reductions of NO_X emissions from specific categories (e.g. ships or construction equipment) may be more effective than across-the-board NO_X reductions. Thus, it is important to remember that the model results described in this section do not define specific requirements for future reductions. They should be interpreted rather as a guide to which types of additional controls will best achieve the goals of the Clean Air Act.

The following tables show the results of the across-the-board reduction scenarios run for each day. Not all possible combinations of reductions were modeled; on August 29-31, peak ozone dropped below 125 parts/billion at reductions of under 50% of both VOC and NO_X, so runs exploring deeper reductions were not necessary. On August 25, additional model runs were necessary to encompass the ozone standard.

Table 2-12 Directional guidance modeling for August 25
(peak ozone concentration in parts/billion)

Aug 25		NO_X reduction %			
VOC reduction %		0	25	50	75
	0	175	168	148	111
	25	154	154	141	109
	50	126	136	130	104
	75	102	107	113	97

Note: Output file for August 25 was post-processed to remove 0700 ozone "spikes" which affected peak concentrations for some combinations of NO_X and VOC reductions.

Table 2-13 Directional guidance modeling for August 29
(peak ozone concentration in parts/billion)

Aug 29	NO_X reduction %			
VOC reduction %		0	25	50
	0	134	137	125
	25	120	123	118
	50	111	107	106

Table 2-14 Directional guidance modeling for August 30
(peak ozone concentration in parts/billion)

Aug 30	NO_X reduction %			
VOC reduction %		0	25	50
	0	144	134	118
	25	135	129	115
	50	123	121	110

Table 2-15 Directional guidance modeling for August 31
(peak ozone concentration in parts/billion)

Aug 31	NO_X reduction %			
VOC reduction %		0	25	50
	0	136	127	114
	25	130	123	111
	50	123	118	108

The directional guidance modeling analysis indicates in all cases that significant additional reductions will be necessary for attainment of the NAAQS, but interestingly show different pathways on different days. On August 25 and 29, the model clearly responds better to VOC reductions, while on August 30 and 31, NO_X reductions appear to provide a faster path to attainment. Of course, targeted reductions of VOC and NO_X will almost certainly prove much more effective than the across-the-board reductions modeled above, and a clear preference for VOC or NO_X reductions may emerge before the Mid-Course Review. For now, though, a combined s1trategy appears to offer a reasonable path to attainment.